# **AUTHOR INDEX TO VOLUME 118**

Alexander, M.H., see D. Lemoine	118 (1987) 357
Alvira, E., L. Vega and C. Girardet, Calculation of chiral discrimination for the	
adsorption of L- and D-alanine molecules on crystalline cellulose	118 (1987) 233
Asada, S., see H. Nakahara	118 (1987) 123
Austin, D.I., R.J. Donovan, A. Hopkirk, K.P. Lawley, D. Shaw and A.J. Yencha,	
Vacuum ultraviolet absorption and fluorescence excitation spectra of Br <sub>2</sub>	118 (1987) 91
Balasubramanian, K., see D.A. Chapman	118 (1987) 333
Beijerinck, H.C.W., see R.J.F. van Gerwen	118 (1987) 407
Bernard, J., M. Hadad and Ph. Kottis, Surface to bulk photodimerisation diffusion in	116 (1967) 407
the crystal of anthracene	118 (1987) 211
	,
Betz, E., see W. Schrof	118 (1987) 57
Bigelow, R.W., see B. Sjögren	118 (1987) 101
Billing, G.D. and G.H.F. Diercksen, Cross sections and rate constants for rotational	110 (1007) 1(1
excitation of NH <sub>3</sub> colliding with $H_2(j=0)$ and $H_2(j=1)$	118 (1987) 161
Browarzik, R.K., see R.D. Kenner	118 (1987) 141
Cao, DZ., see U.K. Roychowdhury	118 (1987) 427
Cavagnat, R.M., see W.G. Rothschild	118 (1987) 33
Chapman, D.A., K. Balasubramanian and S.H. Lin, A theoretical study of spectro-	()
scopic properties and transition moments of HBr	118 (1987) 333
Contreras, R.H., see M.B. Ferraro	118 (1987) 325
Corey, G.C., see D. Lemoine	118 (1987) 357
Corson, M.R., see J.H. LaCasce Jr.	118 (1987) 289
Coxon, J.A., see U.K. Roychowdhury	118 (1987) 427
Coxon, J.A., see O.K. Royenowanary	110 (1707) 427
Dannenberg, J.J., see J.C. Rayez	118 (1987) 265
De Kowalewski, D.G., see M.B. Ferraro	118 (1987) 325
De Lange, C.A., see B.G. Koenders	118 (1987) 113
Derouard, J., see D. Lemoine	118 (1987) 357
Diercksen, G.H.F., see G.D. Billing	118 (1987) 161
Dolan Jr., P.J., see J.H. LaCasce Jr.	118 (1987) 289
Donovan, R.J., see D.I. Austin	118 (1987) 91
Drabe, K.E., see B.G. Koenders	118 (1987) 113
Drchal, V., see S. Záliš	118 (1987) 313
Duguay, B., see J.C. Rayez	118 (1987) 265
Dwyer, J.P., see J.A. Kaye	118 (1987) 153
Elofson, P.A., K. Rynefors and L. Holmlid, Monte Carlo simulation of RRKM	
unimolecular decomposition in molecular beam experiments. V. Product OX angu-	
lar and energy distributions from $O(^3P) + X_2 (X = Br, I)$	118 (1987) 1
Elofson, P.A., see K. Rynefors	118 (1987) 417

Ferraro, M.B., D.G. de Kowalewski, R.H. Contreras and F.S. Ortiz, A theoretical and experimental study of the electric field and magnetic anisotropy effects on proton	
chemical shifts	118 (1987) 325
Flament, J.P., see M. Tadjeddine	118 (1987) 45
Freund, HJ., see B. Sjögren	118 (1987) 101
Freyer, W., see W. Werncke	118 (1987) 133
Fukuda, K., see H. Nakahara	118 (1987) 123
Fukuda, Y., Magnetic field effects on atomic and molecular collisions	118 (1987) 199
Girard, C. and F. Hache, Effective polarizability of a molecule physisorbed on a	
spherical metal particle: nonlocal effects	118 (1987) 249
Girardet, C., see E. Alvira	118 (1987) 233
Guan, Y., see H. Liu	118 (1987) 285
Hache, F., see C. Girard	118 (1987) 249
Hadad, M., see J. Bernard	118 (1987) 211
Haile, J.M., see K.P. Shukla	118 (1987) 241
Halvick, P., see J.C. Rayez	118 (1987) 265
Han, J., see H. Liu	118 (1987) 285
Hikida, T., T. Suzuki and Y. Mori, Fluorescence lifetime studies of NO $A^2\Sigma^+(v=5,$	
$N = 9$ ), $B^2\Pi_{3/2}(v = 8, J = 8.5)$ , $C^2\Pi_{3/2}(v = 1, J = 8.5)$ , $D^2\Sigma^+(v = 0, N = 5)$ and	
$d^2\Sigma^+(v=1, N=9)$	118 (1987) 437
Hiraoka, K. and S. Mizuse, Gas-phase solvation of Cl <sup>-</sup> with H <sub>2</sub> O, CH <sub>3</sub> OH, C <sub>2</sub> H <sub>5</sub> OH,	
$i-C_3H_7OH$ , $n-C_3H_7OH$ , and $t-C_4H_9OH$	118 (1987) 457
Holmlid, L., see P.A. Elofson	118 (1987) 1
Holmlid, L., see K. Rynefors	118 (1987) 417
Hopkirk, A., see D.I. Austin	118 (1987) 91
Humbert, J., see G. Jolicard	118 (1987) 397
Inokuchi, H., see H. Nakahara	118 (1987) 123
Jankowiak, R., G.J. Small and B. Ries, On the density of states for two-level systems in	
amorphous solids	118 (1987) 223
Jaquet, R., Investigations with the finite element method. II. The collinear F + H <sub>2</sub>	
reaction	118 (1987) 17
Jolicard, G. and J. Humbert, Study of the one-channel resonance states. Method	
without a stabilization procedure in the framework of the optical potential model	118 (1987) 397
Kaes, A., see R.D. Kenner	118 (1987) 141
Kalcher, J., Ab initio and pseudopotential investigations on the SiH <sub>n</sub> $(n = 1-3)$	(->)
radicals and their anions	118 (1987) 273
Kanda, K., see H. Nakatsuji	118 (1987) 25
Kaye, J.A., A. Kuppermann and J.P. Dwyer, Quantum-mechanical calculation of the reactions $D + FH(v = 0, 1, 2) \rightarrow DF(v') + H$ and $H + FD(v = 0, 1, 2, 3) \rightarrow HF(v')$	
+ D on a realistic potential energy surface	118 (1987) 153
Kenner, R.D., F. Rohrer, R.K. Browarzik, A. Kaes and F. Stuhl, Two-photon formation of NH/ND(A <sup>3</sup> Π) in the 193 nm photolysis of ammonia. I. Mechanism and	( )
identification of the intermediate species	118 (1987) 141
Kerstel, E.R.T., see R.J.F. van Gerwen	118 (1987) 407
	110 (1701) 401

Kim, M.B., see W. Werncke Koenders, B.G., D.M. Wieringa, K.E. Drabe and C.A. de Lange, A photoelectron	118 (1987) 133
spectroscopy study of low-lying Rydberg states in molecular chlorine using multi-	
photon ionisation	118 (1987) 113
Kottis, Ph., see J. Bernard	118 (1987) 211
Kraemer, W.P. and B.O. Roos, A CAS SCF CI study of the ${}^{1}\Sigma_{g}^{+}$ and ${}^{3}\Pi_{u}$ states of the	
$C_2$ molecule and the ${}^4\Sigma_g$ and ${}^2\Pi_u$ states of the $C_2^+$ ion	118 (1987) 345
Kuppermann, A., see J.A. Kaye	118 (1987) 153
Ruppermann, A., see J.A. Raye	110 (1907) 133
LaCassa Ir III WA Turner M.P. Carson D.I. Dolon Ir and I.V. Nogla Magnetic	
LaCasce Jr., J.H., W.A. Turner, M.R. Corson, P.J. Dolan Jr. and J.K. Nagle, Magnetic	110 (1007) 200
field effects on the luminescence of Cs[Au(CN) <sub>2</sub> ] at low temperatures	118 (1987) 289
Lacey, A.R., see P. Wormell	118 (1987) 71
Lau, A., see W. Werncke	118 (1987) 133
Lawley, K.P., see D.I. Austin	118 (1987) 91
Lemoine, D., G.C. Corey, M.H. Alexander and J. Derouard, Collisional energy transfer involving molecules in <sup>1</sup> Π electronic states: fully quantum study of collisions of	
$\text{Li}_2(\mathbf{B}^1\Pi_{\mu})$ with He and Ne	118 (1987) 357
Leroy, J.P. and R. Wallace, Form of the quantum kinetic energy operator for relative	
motion of a group of particles in a general non-inertial reference frame	118 (1987) 379
Li, S., see H. Liu	118 (1987) 285
	` '
Lin, S.H., see D.A. Chapman	118 (1987) 333
Liu, H., S. Li, J. Han, Y. Guan and C. Wu, Multiphoton ionization and fragmentation	110 (1005) 205
study of acetone at XeCl excimer laser radiation	118 (1987) 285
Mizuse, S., see K. Hiraoka	118 (1987) 457
Mori, Y., see T. Hikida	118 (1987) 437
Moro, G., Coupling of the overall molecular motion with the conformational transi-	
tions. I. The model system of two coupled rotors	118 (1987) 167
Moro, G., Coupling of the overall molecular motion with the conformational transi-	
tions. II. The full rotational problem	118 (1987) 181
	110 (1707) 101
Mrugala, F. and J. Römelt, A generalized log-derivative method for the treatment of	110 (1007) 205
asymmetric collinear reactions in hyperspherical coordinates	118 (1987) 295
Nagle, J.K., see J.H. LaCasce Jr.	118 (1987) 289
Nakahara, H., K. Fukuda, K. Seki, S. Asada and H. Inokuchi, UV photoelectron	
spectroscopic study of the photopolymerization of long-chain diacetylene mono-	
carboxylic acid in Langmuir-Blodgett films	118 (1987) 123
	118 (1987) 25
Nakao, T., see H. Nakatsuji	110 (1907) 23
Nakatsuji, H., T. Nakao and K. Kanda, Electronic mechanism in cadmium chemical	110 (1005) 25
shift	118 (1987) 25
Naxakis, S., see U.K. Roychowdhury	118 (1987) 427
Ortiz, F.S., see M.B. Ferraro	118 (1987) 325
Devet March W.C. Destack 111	110 (1000) 43
Perrot, M., see W.G. Rothschild	118 (1987) 33
Pfeiffer, M., see W. Werncke	118 (1987) 133
Pickard, M.K., see F.A. Smith	118 (1987) 445
Port, H., see W. Schrof	118 (1987) 57
	,

*	
Rayez, J.C., M.T. Rayez, P. Halvick, B. Duguay and J.J. Dannenberg, A theoretical	
study of the decomposition of halogenated alkoxy radicals. II. Fluorine extrusion	118 (1987) 265
Rayez, M.T., see J.C. Rayez	118 (1987) 265
Richards, D.S., see U.K. Roychowdhury	118 (1987) 427
Ries, B., see R. Jankowiak	118 (1987) 223
Rohrer, F., see R.D. Kenner	118 (1987) 141
Römelt, J., see F. Mrugala	118 (1987) 295
Roos, B.O., see W.P. Kraemer	118 (1987) 345
Rothschild, W.G., R.M. Cavagnat and M. Perrot, Vibrational dephasing under frac-	110 (1707) 545
tional ("stretched") exponential modulation in a liquid crystal system	118 (1987) 33
Roychowdhury, U.K., S. Naxakis, J.A. Coxon, D.S. Richards, DZ. Cao and D.W.	110 (1707) 33
Setser, The PF(A $^3\Pi$ -X $^3\Sigma$ -) spectrum from He(2 $^3$ S) + PF <sub>3</sub> : extended vibrational	
analysis and PF(A) vibrational populations	118 (1987) 427
	118 (1987) 427
Rynefors, K., see P.A. Elofson  Rynefors, K. I. Halmiid and P.A. Elofson, Pata constants for reactions O(3P) + V	110 (1907)
Rynefors, K., L. Holmlid and P.A. Elofson, Rate constants for reactions $O(^3P) + X_2 \rightarrow OX + X$ (X = Br, I) determined by an RRKM-type statistical algorithm employ-	
ing Monte Carlo simulation	118 (1987) 417
Salaneck, W.R., see B. Sjögren	118 (1987) 101
Schrof, W., E. Betz, H. Port and H.C. Wolf, Time-resolved fluorescence and sensitized	
fluorescence of orientationally disordered 2,3-dimethylnaphthalene single crystals	118 (1987) 57
Seki, K., see H. Nakahara	118 (1987) 123
Setser, D.W., see U.K. Roychowdhury	118 (1987) 427
Shaw, D., see D.I. Austin	118 (1987) 91
Shukla, K.P. and J.M. Haile, Thermodynamic excess properties from perturbation	
theory. Coupling-parameter approach	118 (1987) 241
Sjögren, B., HJ. Freund, W.R. Salaneck and R.W. Bigelow, Core ionization of	
nitrosobenzene-dimer compounds: phenazon-di-N-oxide	118 (1987) 101
Small, G.J., see R. Jankowiak	118 (1987) 223
Smith, F.A. and M.K. Pickard, Evidence for solute-solute interactions in the inhibition	
of positronium in aqueous solutions	118 (1987) 445
Stuhl, F., see R.D. Kenner	118 (1987) 141
Suzuki, T., see T. Hikida	118 (1987) 437
	()
Tadjeddine, M., J.P. Flament and C. Teichteil, Non-empirical spin-orbit calculation of	
the CH <sub>3</sub> I ground state	118 (1987) 45
Teichteil, C., see M. Tadjeddine	118 (1987) 45
Tschö, J.T., see W. Werncke	118 (1987) 133
Turner, W.A., see J.H. LaCasce Jr.	118 (1987) 289
Van Gerwen, R.J.F., E.J.D. Vredenbregt, E.R.T. Kerstel and H.C.W. Beijerinck, The endothermic excitation transfer process $Kr(^3P_I) + N_2(X) \rightarrow Kr(^1S_0) + N_2(C)$ : a sen-	
sitive probe for the ${}^{3}P_{2}$ : ${}^{3}P_{0}$ population ratio	118 (1987) 407
Vega, L., see E. Alvira	118 (1987) 233
Vredenbregt, E.J.D., see R.J.F. van Gerwen	118 (1987) 407
	110 (1701) 401
Wallace, R., see J.P. Leroy	118 (1987) 379
Weigmann, HJ., see W. Werncke	118 (1987) 133

Werncke, W., A. Lau, M. Pfeiffer, HJ. Weigmann, W. Freyer, J.T. Tschö and M.B. Kim, Transient resonance CARS study on the photoisomerization proces of bis-di-	
methylaminoheptamethine perchlorate (BMC)	118 (1987) 133
Wieringa, D.M., see B.G. Koenders	118 (1987) 113
Wolf, H.C., see W. Schrof	118 (1987) 57
Wormell, P. and A.R. Lacey, Electronic spectra of the naphthyridines: 1,8-naphthyri-	
dine	118 (1987) 71
Wu, C., see H. Liu	118 (1987) 285
Yencha, A.J., see D.I. Austin	118 (1987) 91
Záliš, S. and V. Drchal, A model calculation of redox potential sequence of systems with mutually interacting redox centers: $M(bpy)_3^{(2-n)+}$ systems	118 (1987) 313

#### LIST OF SUBJECTS

#### 1 METHODS

### 1.1 Theoretical

1.1.1	Group	theory	and	algebras	*

- 1.1.2 Classical mechanics \*
- 1.1.3 Quantized field theory \*
- 1.1.4 Many body and quasiparticle approaches
- 1.1.5 Coupling schemes and perturbative treatments
- 1.1.6 Relativistic quantum mechanics \*
- 1.1.7 Transport quantum mechanics \*
- 1.1.8 Equilibrium statistical mechanics \*
- 1.1.9 Statistical mechanics of stationary states \*
- 1.1.10 Non-equilibrium thermodynamic and hydrodynamic theories \*
- 1.1.11 Ab initio schemes for stationary properties
- 1.1.12 Computational and simulation methods
- 1.1.13 Molecular dynamics and scattering theory

## 1.2 Experimental

- 1.2.1 Magnetic resonances
- 1.2.2 Cyclotron resonance \*
- 1.2.3 Microwave spectroscopy \*
- 1.2.4 Infrared spectroscopy \*
- 1.2.5 Raman spectroscopy \*
- 1.2.6 Visible and UV spectroscopy
- 1.2.7 Fluorescence spectroscopy
- 1.2.8 Photoelectron and Auger spectroscopy \*
- 1.2.9 X-ray spectroscopy \*
- 1.2.10 Electron impact spectroscopy \*
- 1.2.11 Laser methods \*
- 1.2.12 Picosecond spectroscopy \*
- 1.2.13 Non-linear optical spectroscopy \*
- 1.2.14 Synchrotron spectroscopies \*
- 1.2.15 Coherent optical spectroscopy \*
- 1.2.16 Optical pumping \*
- 1.2.17 Multiple resonance spectroscopy \*
- 1.2.18 Optoacoustic spectroscopy \*
- 1.2.19 Atomic and molecular beam techniques
- 1.2.20 Time-resolved experiments
- 1.2.21 Mass spectrometry
- 1.2.22 Radiolysis \*
- 1.2.23 Mössbauer spectroscopy \*
- 1.2.24 X-ray, electron and neutron diffraction \*
- 1.2.25 Neutron scattering \*
- 1.2.26 Light scattering \*
- 1.2.27 Field emission and field ionization \*
- 1.2.28 Measurement of macroscopic variables \*

### 2 OBJECTS

### 2.1 Bulk systems

- 2.1.1 Gases
- 2.1.2 Supersonic beams \*
- 2.1.3 Liquids neat \*
- 2.1.4 Liquid mixtures and solutions
- 2.1.5 Crystals \*
- 2.1.5.1 neat \*
- 2.1.5.2 mixed \*
- 2.1.6 Glasses \*
- 2.1.7 Liquid crystals \*
- 2.1.8 Polymers \*
- 2.1.9 Semiconductors \*
- 2.1.10 Metals and alloys \*
- 2.1.11 Thin films \*
- 2.1.12 Surfaces \*
- 2.1.13 Low-dimensional materials \*
- 2.1.14 Dielectrics \*
- 2.1.15 Plasmas \*
- 2.1.16 Biological systems \*

## 2.2 Microscopic systems

- 2.2.1 Atoms \*
- 2.2.2 Molecules (neutral and ionic) \*
- 2.2.2.1 diatomic
- 2.2.2.2 small polyatomics
- 2.2.2.3 aromatics \*
- 2.2.2.4 other large \*
- 2.2.2.5 polymeric and biological \*
- 2.2.3 Molecular aggregates
- 2.2.3.1 dimers \*
- 2.2.3.2 van der Waals molecules \*
- 2.2.3.3 clusters \*
- 2.2.3.4 complexes
- 2.2.4 Free radicals (including hydronium and muonium)
- 2.2.5 Quasiparticles (including excitons) \*
- 2.2.6 Defects and impurities \*
- 2.2.7 Ions and charge carriers \*

<sup>\*</sup> Denotes subject not covered in this volume.

## 3 PHENOMENA

3.1	Molecular structure	3.16	Multiphoton phenomena *
3.2	Vibrations and rotations of molecules	3.17	Reactions (including dissociation) *
3.3	Electronic structure and states	3.17.1	gas phase
3.4	Electric and magnetic properties *	3.17.2	condensed phase
3.5	Spin splittings *	3.17.3	photochemical *
3.6	Optical activity *	3.18	Tunnelling
3.7	Molecular interactions	3.19	Electron transfer *
3.8	Spectral bandshapes and intensities	3.20	Positron annihilation
3.9	Coupling of electronic and nuclear motion *	3.21	Ionization (including Rydberg states) *
3.10	Energy transfer processes	3.22	Molecular motion (including diffusive) *
3.11	Molecular photophysical processes *	3.23	Isotopic effects *
3.12	Intramolecular dynamics	3.24	Fluctuations and noise *
3.12.1	radiationless transitions *	3.25	Collective motion and excitations *
3.12.2	vibrational energy distribution	3.26	Surface effects and catalysis *
	(including vibrational dissociation) *	3.27	Thermodynamic and transport properties *
3.13	Luminescence spectra, yields and lifetimes *	3.28	Structure of solids and liquids
3.14	Coherence loss processes *	3.29	Critical phenomena *
3.15	Non-linear responses (including optical) *	3.30	Phase transitions *

## **SUBJECT INDEX TO VOLUME 118**

# **METHODS**

# Theoretical

Quantized field theory Surface to bulk photodimerisation diffusion in the crystal of anthracene, J. Bernard, M. Hadad and Ph. Kottis	118 (1987) 211
Many body and quasiparticle approaches  Core ionization of nitrosobenzene-dimer compounds: phenazon-di-N-oxide, B. Sjögren,  HJ. Freund, W.R. Salaneck and R.W. Bigelow	118 (1987) 101
Effective polarizability of a molecule physisorbed on a spherical metal particle: nonlocal effects, C. Girard and F. Hache  A model calculation of redox potential sequence of systems with mutually interacting	118 (1987) 249
redox centers: $M(bpy)_3^{(2-n)+}$ systems, S. Záliš and V. Drchal Coupling schemes and perturbative treatments	118 (1987) 313
Vibrational dephasing under fractional ("stretched") exponential modulation in a liquid crystal system, W.G. Rothschild, R.M. Cavagnat and M. Perrot Non-empirical spin-orbit calculation of the CH <sub>3</sub> I ground state, M. Tadjeddine, J.P.	118 (1987) 33
Flament and C. Teichteil  A theoretical and experimental study of the electric field and magnetic anisotropy effects on proton chemical shifts, M.B. Ferraro, D.G. de Kowalewski, R.H. Contreras and F.S. Ortiz	118 (1987) 45 118 (1987) 325
Relativistic quantum mechanics  Non-empirical spin-orbit calculation of the CH <sub>3</sub> I ground state, M. Tadjeddine, J.P. Flament and C. Teichteil  A theoretical study of spectroscopic properties and transition moments of HBr, D.A.	118 (1987) 45
Chapman, K. Balasubramanian and S.H. Lin	118 (1987) 333
Equilibrium statistical mechanics  Thermodynamic excess properties from perturbation theory. Coupling-parameter approach, K.P. Shukla and J.M. Haile	118 (1987) 241
Ab initio schemes for stationary properties  Electronic mechanism in cadmium chemical shift, H. Nakatsuji, T. Nakao and K. Kanda	118 (1987) 25
Non-empirical spin-orbit calculation of the CH <sub>3</sub> I ground state, M. Tadjeddine, J.P. Flament and C. Teichteil  A theoretical study of the decomposition of halogenated alkoxy radicals. II. Fluorine	118 (1987) 45
extrusion, J.C. Rayez, M.T. Rayez, P. Halvick, B. Duguay and J.J. Dannenberg	118 (1987) 265

Ab initio and pseudopotential investigations on the $SiH_n$ ( $n = 1-3$ ) radicals and their	
anions, J. Kalcher	118 (1987) 273
A theoretical study of spectroscopic properties and transition moments of HBr, D.A.	
Chapman, K. Balasubramanian and S.H. Lin	118 (1987) 333
A CAS SCF CI study of the ${}^{1}\Sigma_{g}^{+}$ and ${}^{3}\Pi_{u}$ states of the $C_{2}$ molecule and the ${}^{4}\Sigma_{g}$ and	(,
$^{2}\Pi_{u}$ states of the $C_{2}^{+}$ ion, W.P. Kraemer and B.O. Roos	118 (1987) 345
Computational and simulation methods	
Monte Carlo simulation of RRKM unimolecular decomposition in molecular beam	
experiments. V. Product OX angular and energy distributions from $O(^3P) + X_2$	
(X = Br, I), P.A. Elofson, K. Rynefors and L. Holmlid	118 (1987) 1
Investigations with the finite element method. II. The collinear F + H <sub>2</sub> reaction, R.	
Jaquet	118 (1987) 17
Electronic mechanism in cadmium chemical shift, H. Nakatsuji, T. Nakao and K.	
Kanda	118 (1987) 25
Surface to bulk photodimerisation diffusion in the crystal of anthracene, J. Bernard,	()
M. Hadad and Ph. Kottis	118 (1987) 211
On the density of states for two-level systems in amorphous solids, R. Jankowiak, G.J.	110 (1707) 211
Small and B. Ries	118 (1987) 223
Calculation of chiral discrimination for the adsorption of L- and D-alanine molecules	110 (1707) 223
on crystalline cellulose, E. Alvira, L. Vega and C. Girardet	118 (1987) 233
A generalized log-derivative method for the treatment of asymmetric collinear reac-	110 (1907) 233
	110 (1007) 205
tions in hyperspherical coordinates, F. Mrugala and J. Römelt	118 (1987) 295
Collisional energy transfer involving molecules in <sup>1</sup> $\Pi$ electronic states: fully quantum	
study of collisions of $\text{Li}_2(B^1\Pi_u)$ with He and Ne, D. Lemoine, G.C. Corey, M.H.	110 (1007) 257
Alexander and J. Derouard	118 (1987) 357
Molecular describes and continue there.	
Molecular dynamics and scattering theory	
Monte Carlo simulation of RRKM unimolecular decomposition in molecular beam	
experiments. V. Product OX angular and energy distributions from $O(^3P) + X_2$	110 (1007) 1
(X = Br, I), P.A. Elofson, K. Rynefors and L. Holmlid	118 (1987) 1
Investigations with the finite element method. II. The collinear $F + H_2$ reaction, R.	110 (1005) 15
Jaquet	118 (1987) 17
Vibrational dephasing under fractional ("stretched") exponential modulation in a	
liquid crystal system, W.G. Rothschild, R.M. Cavagnat and M. Perrot	118 (1987) 33
Quantum-mechanical calculation of the reactions $D + FH(v = 0, 1, 2) \rightarrow DF(v') + H$	
and H + FD( $v = 0, 1, 2, 3$ ) $\rightarrow$ HF( $v'$ ) + D on a realistic potential energy surface,	
J.A. Kaye, A. Kuppermann and J.P. Dwyer	118 (1987) 153
Cross sections and rate constants for rotational excitation of NH <sub>3</sub> colliding with	
$H_2(j=0)$ and $H_2(j=1)$ , G.D. Billing and G.H.F. Diercksen	118 (1987) 161
Coupling of the overall molecular motion with the conformational transitions. I. The	
model system of two coupled rotors, G. Moro	118 (1987) 167
Coupling of the overall molecular motion with the conformational transitions. II. The	
full rotational problem, G. Moro	118 (1987) 181
Magnetic field effects on atomic and molecular collisions, Y. Fukuda	118 (1987) 199
Collisional energy transfer involving molecules in <sup>1</sup> $\Pi$ electronic states: fully quantum	
Comsional energy transfer involving molecules in 11 electronic states, runy quantum	
study of collisions of $\text{Li}_2(B^1\Pi_u)$ with He and Ne, D. Lemoine, G.C. Corey, M.H. Alexander and J. Derouard	118 (1987) 357

particles in a general non-inertial refere	perator for relative motion of a group of nce frame, J.P. Leroy and R. Wallace  Method without a stabilization procedure in	118 (1987) 379
the framework of the optical potential r The endothermic excitation transfer proc	model, G. Jolicard and J. Humbert ess $Kr(^3P_J) + N_2(X) \rightarrow Kr(^1S_0) + N_2(C)$ : a	118 (1987) 397
Vredenbregt, E.R.T. Kerstel and H.C.W. Rate constants for reactions $O(^3P) + X_2$	$\rightarrow$ OX + X (X = Br, I) determined by an	118 (1987) 407
L. Holmlid and P.A. Elofson	ying Monte Carlo simulation, K. Rynefors,	118 (1987) 417
Experimental		
	the electric field and magnetic anisotropy Ferraro, D.G. de Kowalewski, R.H. Con-	
treras and F.S. Ortiz	Torrate, previous remaining remaining	118 (1987) 325
Raman spectroscopy		
liquid crystal system, W.G. Rothschild, Transient resonance CARS study on the	photoisomerization proces of bis-dimethyl-	118 (1987) 33
weigmann, W. Freyer, J.T. Tschö and M	, W. Werncke, A. Lau, M. Pfeiffer, HJ. M.B. Kim	118 (1987) 133
Visible and UV spectroscopy	10 - 1d - '1' D W - 11 - 1 A D	
Lacey	1,8-naphthyridine, P. Wormell and A.R.	118 (1987) 71
Surface to bulk photodimerisation diffusion M. Hadad and Ph. Kottis	on in the crystal of anthracene, J. Bernard,	118 (1987) 211
	(2 <sup>3</sup> S) + PF <sub>3</sub> : extended vibrational analysis L. Roychowdhury, S. Naxakis, J.A. Coxon,	
D.S. Richards, DZ. Cao and D.W. Sets		118 (1987) 427
Fluorescence spectroscopy		
2,3-dimethylnaphthalene single crystals,	fluorescence of orientationally disordered W. Schrof, E. Betz, H. Port and H.C. Wolf 1,8-naphthyridine, P. Wormell and A.R.	118 (1987) 57
Lacey		118 (1987) 71
$C^2\Pi_{3/2}(v=1,\ J=8.5),\ D^2\Sigma^+(v=0,\ I$ T. Suzuki and Y. Mori	$\Sigma^{+}(v=5, N=9), \ B^{2}\Pi_{3/2}(v=8, J=8.5),$ $N=5) \text{ and } d^{2}\Sigma^{+}(v=1, N=9), \text{ T. Hikida},$	118 (1987) 437
Photoelectron and Auger spectroscopy		
Core ionization of nitrosobenzene-dimer con	mpounds: phenazon-di-N-oxide, B. Sjögren,	440 (400=) 404
	Bigelow -lying Rydberg states in molecular chlorine ders, D.M. Wieringa, K.E. Drabe and C.A.	118 (1987) 101
de Lange		118 (1987) 113

UV photoelectron spectroscopic study of the photopolymerization of long-chain diacetylene monocarboxylic acid in Langmuir-Blodgett films, H. Nakahara, K. Fukuda, K. Seki, S. Asada and H. Inokuchi	118 (1987) 123
Laser methods Two-photon formation of NH/ND(A³Π) in the 193 nm photolysis of ammonia. I. Mechanism and identification of the intermediate species, R.D. Kenner, F. Rohrer, R.K. Browarzik, A. Kaes and F. Stuhl	118 (1987) 141
Picosecond spectroscopy Time-resolved fluorescence and sensitized fluorescence of orientationally disordered 2,3-dimethylnaphthalene single crystals, W. Schrof, E. Betz, H. Port and H.C. Wolf	118 (1987) 57
Synchrotron spectroscopies  Vacuum ultraviolet absorption and fluorescence excitation spectra of Br <sub>2</sub> , D.I. Austin,  R.J. Donovan, A. Hopkirk, K.P. Lawley, D. Shaw and A.J. Yencha	118 (1987) 91
Multiple resonance spectroscopy  Multiphoton ionization and fragmentation study of acetone at XeCl excimer laser radiation, H. Liu, S. Li, J. Han, Y. Guan and C. Wu	118 (1987) 285
<ul> <li>Atomic and molecular beam techniques</li> <li>Multiphoton ionization and fragmentation study of acetone at XeCl excimer laser radiation, H. Liu, S. Li, J. Han, Y. Guan and C. Wu</li> <li>The endothermic excitation transfer process Kr(<sup>3</sup>P<sub>J</sub>) + N<sub>2</sub>(X) → Kr(<sup>1</sup>S<sub>0</sub>) + N<sub>2</sub>(C): a sensitive probe for the <sup>3</sup>P<sub>2</sub>: <sup>3</sup>P<sub>0</sub> population ratio, R.J.F. van Gerwen, E.J.D. Vredenbregt, E.R.T. Kerstel and H.C.W. Beijerinck</li> </ul>	118 (1987) 285 118 (1987) 407
Time-resolved experiments  Transient resonance CARS study on the photoisomerization proces of bis-dimethylaminoheptamethine perchlorate (BMC), W. Werncke, A. Lau, M. Pfeiffer, HJ. Weigmann, W. Freyer, J.T. Tschö and M.B. Kim  Two-photon formation of NH/ND(A³Π) in the 193 nm photolysis of ammonia. I. Mechanism and identification of the intermediate species, R.D. Kenner, F. Rohrer, R.K. Browarzik, A. Kaes and F. Stuhl  Magnetic field effects on the luminescence of Cs[Au(CN) <sub>2</sub> ] at low temperatures, J.H. LaCasce Jr., W.A. Turner, M.R. Corson, P.J. Dolan Jr. and J.K. Nagle  Fluorescence lifetime studies of NO A²Σ⁺(v = 5, N = 9), B²Π <sub>3/2</sub> (v = 8, J = 8.5), C²Π <sub>3/2</sub> (v = 1, J = 8.5), D²Σ⁺(v = 0, N = 5) and d²Σ⁺(v = 1, N = 9), T. Hikida,	118 (1987) 133 118 (1987) 141 118 (1987) 289
T. Suzuki and Y. Mori Evidence for solute-solute interactions in the inhibition of positronium in aqueous solutions, F.A. Smith and M.K. Pickard	118 (1987) 437 118 (1987) 445
Mass spectrometry Gas-phase solvation of Cl <sup>-</sup> with H <sub>2</sub> O, CH <sub>3</sub> OH, C <sub>2</sub> H <sub>5</sub> OH, i-C <sub>3</sub> H <sub>7</sub> OH, n-C <sub>3</sub> H <sub>7</sub> OH, and t-C <sub>4</sub> H <sub>9</sub> OH, K. Hiraoka and S. Mizuse	118 (1987) 457

## **OBJECTS**

# **Bulk systems**

Gases	
A photoelectron spectroscopy study of low-lying Rydberg states in molecular chlorine using multiphoton ionisation, B.G. Koenders, D.M. Wieringa, K.E. Drabe and C.A.	
de Lange	118 (1987) 113
Two-photon formation of NH/ND(A <sup>3</sup> II) in the 193 nm photolysis of ammonia. I.	110 (1707) 11.
Mechanism and identification of the intermediate species, R.D. Kenner, F. Rohrer,	110 (1007) 141
R.K. Browarzik, A. Kaes and F. Stuhl A theoretical study of the decomposition of halogenated alkoxy radicals. II. Fluorine	118 (1987) 141
extrusion, J.C. Rayez, M.T. Rayez, P. Halvick, B. Duguay and J.J. Dannenberg	118 (1987) 265
Fluorescence lifetime studies of NO A <sup>2</sup> $\Sigma^+$ ( $v = 5$ , $N = 9$ ), B <sup>2</sup> $\Pi_{3/2}$ ( $v = 8$ , $J = 8.5$ ),	110 (1707) 200
$C^2\Pi_{3/2}(v=1,\ J=8.5),\ D^2\Sigma^+(v=0,\ N=5)$ and $d^2\Sigma^+(v=1,\ N=9),\ T.$ Hikida, T. Suzuki and Y. Mori	118 (1987) 437
Gas-phase solvation of Cl <sup>-</sup> with H <sub>2</sub> O, CH <sub>3</sub> OH, C <sub>2</sub> H <sub>5</sub> OH, <i>i</i> -C <sub>3</sub> H <sub>7</sub> OH, <i>n</i> -C <sub>3</sub> H <sub>7</sub> OH,	110 (1707) 437
and $t$ -C <sub>4</sub> H <sub>9</sub> OH, K. Hiraoka and S. Mizuse	118 (1987) 457
Liquid mixtures and solutions	
Transient resonance CARS study on the photoisomerization proces of bis-dimethyl-	
aminoheptamethine perchlorate (BMC), W. Werncke, A. Lau, M. Pfeiffer, HJ.	110 (1007) 123
Weigmann, W. Freyer, J.T. Tschö and M.B. Kim Thermodynamic excess properties from perturbation theory. Coupling-parameter ap-	118 (1987) 133
proach, K.P. Shukla and J.M. Haile	118 (1987) 241
Evidence for solute-solute interactions in the inhibition of positronium in aqueous	110 (1707) 241
solutions, F.A. Smith and M.K. Pickard	118 (1987) 445
Crystals	
Time-resolved fluorescence and sensitized fluorescence of orientationally disordered 2,3-dimethylnaphthalene single crystals, W. Schrof, E. Betz, H. Port and H.C. Wolf	118 (1987) 57
– neat	
Surface to bulk photodimerisation diffusion in the crystal of anthracene, J. Bernard,	
M. Hadad and Ph. Kottis	118 (1987) 211
- mixed	
Electronic spectra of the naphthyridines: 1,8-naphthyridine, P. Wormell and A.R.	
Lacey	118 (1987) 71
Magnetic field effects on the luminescence of Cs[Au(CN) <sub>2</sub> ] at low temperatures, J.H. LaCasce Jr., W.A. Turner, M.R. Corson, P.J. Dolan Jr. and J.K. Nagle	118 (1987) 289
Glasses	
On the density of states for two-level systems in amorphous solids, R. Jankowiak, G.J.	
Small and B. Ries	118 (1987) 223
Liquid crystals	
Vibrational dephasing under fractional ("stretched") exponential modulation in a	
liquid crystal system, W.G. Rothschild, R.M. Cavagnat and M. Perrot.	118 (1987) 33

Metals and alloys  Effective polarizability of a molecule physisorbed on a spherical metal particle: nonlocal effects, C. Girard and F. Hache	118 (1987) 249
Thin films  Core ionization of nitrosobenzene-dimer compounds: phenazon-di-N-oxide, B. Sjögren, HJ. Freund, W.R. Salaneck and R.W. Bigelow  UV photoelectron spectroscopic study of the photopolymerization of long-chain diacetylene monocarboxylic acid in Langmuir-Blodgett films, H. Nakahara, K.	118 (1987) 101
Fukuda, K. Seki, S. Asada and H. Inokuchi  Microscopic systems	118 (1987) 123
Microscopic systems	
Atoms  Magnetic field effects on atomic and molecular collisions, Y. Fukuda	118 (1987) 199
Thermodynamic excess properties from perturbation theory. Coupling-parameter approach, K.P. Shukla and J.M. Haile	118 (1987) 241
Molecules (neutral and ionic)	
Magnetic field effects on atomic and molecular collisions, Y. Fukuda	118 (1987) 199
- diatomic	
Vacuum ultraviolet absorption and fluorescence excitation spectra of Br <sub>2</sub> , D.I. Austin, R.J. Donovan, A. Hopkirk, K.P. Lawley, D. Shaw and A.J. Yencha	118 (1987) 91
A photoelectron spectroscopy study of low-lying Rydberg states in molecular chlorine using multiphoton ionisation, B.G. Koenders, D.M. Wieringa, K.E. Drabe and C.A.	110 (1007) 112
de Lange Cross sections and rate constants for rotational excitation of NH <sub>3</sub> colliding with	118 (1987) 113
$H_2(j=0)$ and $H_2(j=1)$ , G.D. Billing and G.H.F. Diercksen	118 (1987) 161
A theoretical study of spectroscopic properties and transition moments of HBr, D.A. Chapman, K. Balasubramanian and S.H. Lin	118 (1987) 333
A CAS SCF CI study of the ${}^{1}\Sigma_{g}^{+}$ and ${}^{3}\Pi_{u}$ states of the $C_{2}$ molecule and the ${}^{4}\Sigma_{g}$ and	110 (1007) 245
$^2\Pi_{\rm u}$ states of the ${\rm C_2^+}$ ion, W.P. Kraemer and B.O. Roos Collisional energy transfer involving molecules in $^1\Pi$ electronic states: fully quantum	118 (1987) 345
study of collisions of Li <sub>2</sub> (B <sup>1</sup> Π <sub>u</sub> ) with He and Ne, D. Lemoine, G.C. Corey, M.H.	110 (1007) 257
Alexander and J. Derouard The endothermic excitation transfer process $Kr(^{3}P_{J}) + N_{2}(X) \rightarrow Kr(^{1}S_{0}) + N_{2}(C)$ : a	118 (1987) 357
sensitive probe for the <sup>3</sup> P <sub>2</sub> : <sup>3</sup> P <sub>0</sub> population ratio, R.J.F. van Gerwen, E.J.D.	110 (1007) 407
Vredenbregt, E.R.T. Kerstel and H.C.W. Beijerinck The PF(A <sup>3</sup> $\Pi$ -X <sup>3</sup> $\Sigma$ <sup>-</sup> ) spectrum from He(2 <sup>3</sup> S) + PF <sub>3</sub> : extended vibrational analysis	118 (1987) 407
and PF(A) vibrational populations, U.K. Roychowdhury, S. Naxakis, J.A. Coxon,	110 (1007) 437
D.S. Richards, DZ. Cao and D.W. Setser Fluorescence lifetime studies of NO A <sup>2</sup> $\Sigma^+(v=5, N=9)$ , B <sup>2</sup> $\Pi_{3/2}(v=8, J=8.5)$ ,	118 (1987) 427
$C^2\Pi_{3/2}(v=1,\ J=8.5),\ D^2\Sigma^+(v=0,\ N=5)$ and $d^2\Sigma^+(v=1,\ N=9),\ T.$ Hikida, T. Suzuki and Y. Mori	118 (1987) 437
- small polyatomics	
Non-empirical spin-orbit calculation of the CH <sub>3</sub> I ground state, M. Tadjeddine, J.P. Flament and C. Teichteil	118 (1987) 45

Cross sections and rate constants for rotational excitation of NH <sub>3</sub> colliding with $H_2(j=0)$ and $H_2(j=1)$ , G.D. Billing and G.H.F. Diercksen	118 (1987) 161
A theoretical study of the decomposition of halogenated alkoxy radicals. II. Fluorine extrusion, J.C. Rayez, M.T. Rayez, P. Halvick, B. Duguay and J.J. Dannenberg Ab initio and pseudopotential investigations on the $SiH_n$ ( $n = 1-3$ ) radicals and their anions, J. Kalcher	118 (1987) 265
	118 (1987) 273
Multiphoton ionization and fragmentation study of acetone at XeCl excimer laser radiation, H. Liu, S. Li, J. Han, Y. Guan and C. Wu  A theoretical and experimental study of the electric field and magnetic anisotropy	118 (1987) 285
effects on proton chemical shifts, M.B. Ferraro, D.G. de Kowalewski, R.H. Contreras and F.S. Ortiz	118 (1987) 325
Form of the quantum kinetic energy operator for relative motion of a group of particles in a general non-inertial reference frame, J.P. Leroy and R. Wallace	118 (1987) 379
- aromatics Time-resolved fluorescence and sensitized fluorescence of orientationally disordered	
2,3-dimethylnaphthalene single crystals, W. Schrof, E. Betz, H. Port and H.C. Wolf Core ionization of nitrosobenzene-dimer compounds: phenazon-di-N-oxide, B. Sjögren,	118 (1987) 57
HJ. Freund, W.R. Salaneck and R.W. Bigelow Surface to bulk photodimerisation diffusion in the crystal of anthracene, J. Bernard,	118 (1987) 101
M. Hadad and Ph. Kottis	118 (1987) 211
- other large Electronic mechanism in cadmium chemical shift, H. Nakatsuji, T. Nakao and K. Kanda	118 (1987) 25
<ul> <li>polymeric and biological</li> <li>UV photoelectron spectroscopic study of the photopolymerization of long-chain diacetylene monocarboxylic acid in Langmuir-Blodgett films, H. Nakahara, K.</li> </ul>	
Fukuda, K. Seki, S. Asada and H. Inokuchi Calculation of chiral discrimination for the adsorption of L- and D-alanine molecules	118 (1987) 123
on crystalline cellulose, E. Alvira, L. Vega and C. Girardet	118 (1987) 233
Molecular aggregates Gas-phase solvation of Cl <sup>-</sup> with H <sub>2</sub> O, CH <sub>3</sub> OH, C <sub>2</sub> H <sub>5</sub> OH, <i>i</i> -C <sub>3</sub> H <sub>7</sub> OH, <i>n</i> -C <sub>3</sub> H <sub>7</sub> OH, and <i>t</i> -C <sub>4</sub> H <sub>9</sub> OH, K. Hiraoka and S. Mizuse	118 (1987) 457
-clusters  Magnetic field effects on the luminescence of Cs[Au(CN) <sub>2</sub> ] at low temperatures, J.H. LaCasce Jr., W.A. Turner, M.R. Corson, P.J. Dolan Jr. and J.K. Nagle	118 (1987) 289
-complexes  Monte Carlo simulation of RRKM unimolecular decomposition in molecular beam experiments. V. Product OX angular and energy distributions from O( <sup>3</sup> P) + X <sub>2</sub>	110 (1007)
(X = Br, I), P.A. Elofson, K. Rynefors and L. Holmlid  A model calculation of redox potential sequence of systems with mutually interacting	118 (1987) 1
redox centers: $M(bpy)_3^{(2-n)+}$ systems, S. Záliš and V. Drchal	118 (1987) 313

Rate constants for reactions $O(^3P) + X_2 \rightarrow OX + X$ (X = Br, I) determine RRKM-type statistical algorithm employing Monte Carlo simulation, K. L. Holmlid and P.A. Elofson	
<ul> <li>Free radicals (including hydronium and muonium)</li> <li>Monte Carlo simulation of RRKM unimolecular decomposition in molecular experiments. V. Product OX angular and energy distributions from OX (X = Br, I), P.A. Elofson, K. Rynefors and L. Holmlid</li> <li>Two-photon formation of NH/ND(A³Π) in the 193 nm photolysis of an Mechanism and identification of the intermediate species, R.D. Kenner, I.</li> </ul>	118 (1987) 1 nmonia. I.
R.K. Browarzik, A. Kaes and F. Stuhl	118 (1987) 141
A theoretical study of the decomposition of halogenated alkoxy radicals. Il extrusion, J.C. Rayez, M.T. Rayez, P. Halvick, B. Duguay and J.J. Danne	enberg 118 (1987) 265
Ab initio and pseudopotential investigations on the SiH <sub>n</sub> $(n = 1-3)$ radicals anions, J. Kalcher	118 (1987) 273
Evidence for solute-solute interactions in the inhibition of positronium is solutions, F.A. Smith and M.K. Pickard	118 (1987) 445
PHENOMENA	
Molecular structure	
Transient resonance CARS study on the photoisomerization proces of bis aminoheptamethine perchlorate (BMC), W. Werncke, A. Lau, M. Pfei Weigmann, W. Freyer, J.T. Tschö and M.B. Kim  A theoretical and experimental study of the electric field and magnetic a effects on proton chemical shifts, M.B. Ferraro, D.G. de Kowalewski, I	ffer, HJ. 118 (1987) 133 anisotropy
treras and F.S. Ortiz	118 (1987) 325
Vibrations and rotations of molecules A CAS SCF CI study of the $^1\Sigma_g^+$ and $^3\Pi_u$ states of the $C_2$ molecule and the $^2\Pi_u$ states of the $C_2^+$ ion, W.P. Kraemer and B.O. Roos	118 (1987) 345
Form of the quantum kinetic energy operator for relative motion of a particles in a-general non-inertial reference frame, J.P. Leroy and R. Wal The PF(A $^3\Pi$ -X $^3\Sigma$ -) spectrum from He(2 $^3$ S) + PF <sub>3</sub> : extended vibrational	lace 118 (1987) 379
and PF(A) vibrational populations, U.K. Roychowdhury, S. Naxakis, J. D.S. Richards, DZ. Cao and D.W. Setser	
Electronic structure and states Electronic mechanism in cadmium chemical shift, H. Nakatsuji, T. Naka Kanda	o and K.  118 (1987) 25
Non-empirical spin-orbit calculation of the CH <sub>3</sub> I ground state, M. Tadjec Flament and C. Teichteil	ldine, J.P. 118 (1987) 45
Electronic spectra of the naphthyridines: 1,8-naphthyridine, P. Wormell Lacey	and A.R. 118 (1987) 71
Vacuum ultraviolet absorption and fluorescence excitation spectra of Br <sub>2</sub> , D R.J. Donovan, A. Hopkirk, K.P. Lawley, D. Shaw and A.J. Yencha	
Core ionization of nitrosobenzene-dimer compounds: phenazon-di-N-oxide, I HJ. Freund, W.R. Salaneck and R.W. Bigelow	
,	, , , , , , , , , , , , , , , , , , , ,

A photoelectron spectroscopy study of low-lying Rydberg states in molecusing multiphoton ionisation, B.G. Koenders, D.M. Wieringa, K.E. Dr. de Lange  UV photoelectron spectroscopic study of the photopolymerization of le	abe and C.A. 118 (1987) 113 ong-chain di-
acetylene monocarboxylic acid in Langmuir-Blodgett films, H. N Fukuda, K. Seki, S. Asada and H. Inokuchi	118 (1987) 123
On the density of states for two-level systems in amorphous solids, R. Jan Small and B. Ries	118 (1987) 223
Ab initio and pseudopotential investigations on the SiH <sub>n</sub> $(n = 1-3)$ radio anions, J. Kalcher	118 (1987) 273
A model calculation of redox potential sequence of systems with mutual redox centers: $M(bpy)_3^{(2-n)+}$ systems, S. Záliš and V. Drchal	118 (1987) 313
A theoretical study of spectroscopic properties and transition moments of Chapman, K. Balasubramanian and S.H. Lin	118 (1987) 333
Electric and magnetic properties	
Electronic mechanism in cadmium chemical shift, H. Nakatsuji, T. N Kanda	118 (1987) 25
Calculation of chiral discrimination for the adsorption of L- and D-aland on crystalline cellulose, E. Alvira, L. Vega and C. Girardet  Magnetic field effects on the luminescence of ColAv(CN), let low temperature of ColAv(CN).	118 (1987) 233
Magnetic field effects on the luminescence of Cs[Au(CN) <sub>2</sub> ] at low temporal LaCasce Jr., W.A. Turner, M.R. Corson, P.J. Dolan Jr. and J.K. Nagle	
Molecular interactions	
Magnetic field effects on atomic and molecular collisions, Y. Fukuda Surface to bulk photodimerisation diffusion in the crystal of anthracene	
M. Hadad and Ph. Kottis  Calculation of chiral discrimination for the adsorption of L- and D-alani	118 (1987) 211 ne molecules
on crystalline cellulose, E. Alvira, L. Vega and C. Girardet Gas-phase solvation of Cl <sup>-</sup> with H <sub>2</sub> O, CH <sub>3</sub> OH, C <sub>2</sub> H <sub>5</sub> OH, <i>i</i> -C <sub>3</sub> H <sub>7</sub> OH,	118 (1987) 233 <i>n</i> -C <sub>3</sub> H <sub>7</sub> OH,
and t-C <sub>4</sub> H <sub>9</sub> OH, K. Hiraoka and S. Mizuse	118 (1987) 457
Spectral bandshapes and intensities	-CIID- DA
A theoretical study of spectroscopic properties and transition moments of Chapman, K. Balasubramanian and S.H. Lin  The PF(A $^{3}\Pi$ -X $^{3}\Sigma$ -) spectrum from He(2 $^{3}$ S) + PF <sub>3</sub> : extended vibration	118 (1987) 333
and PF(A) vibrational populations, U.K. Roychowdhury, S. Naxakis, D.S. Richards, DZ. Cao and D.W. Setser	
Energy transfer processes	
Investigations with the finite element method. II. The collinear $F + H_2$ Jaquet	reaction, R. 118 (1987) 17
Time-resolved fluorescence and sensitized fluorescence of orientationall 2,3-dimethylnaphthalene single crystals, W. Schrof, E. Betz, H. Port and	
Cross sections and rate constants for rotational excitation of NH <sub>3</sub> con $H_2(j=0)$ and $H_2(j=1)$ , G.D. Billing and G.H.F. Diercksen	
Collisional energy transfer involving molecules in ${}^{1}\Pi$ electronic states: further study of collisions of $\text{Li}_{2}(B^{1}\Pi_{11})$ with He and Ne, D. Lemoine, G.C.	ally quantum
Alexander and J. Derouard	118 (1987) 357

	100
The endothermic excitation transfer process $Kr(^3P_J) + N_2(X) \rightarrow Kr(^1S_0) + N_2(C)$ : a sensitive probe for the $^3P_2$ : $^3P_0$ population ratio, R.J.F. van Gerwen, E.J.D. Vredenbregt, E.R.T. Kerstel and H.C.W. Beijerinck	118 (1987) 407
Molecular photophysical processes	
Transient resonance CARS study on the photoisomerization proces of bis-dimethyl-aminoheptamethine perchlorate (BMC), W. Werncke, A. Lau, M. Pfeiffer, HJ. Weigmann, W. Freyer, J.T. Tschö and M.B. Kim	118 (1987) 133
Intramolecular dynamics	
Coupling of the overall molecular motion with the conformational transitions. I. The model system of two coupled rotors, G. Moro	118 (1987) 167
Coupling of the overall molecular motion with the conformational transitions. II. The full rotational problem, G. Moro	118 (1987) 181
Form of the quantum kinetic energy operator for relative motion of a group of	110 (1907) 101
particles in a general non-inertial reference frame, J.P. Leroy and R. Wallace Study of the one-channel resonance states. Method without a stabilization procedure in	118 (1987) 379
the framework of the optical potential model, G. Jolicard and J. Humbert	118 (1987) 397
Non-linear responses (including optical)  Effective polarizability of a molecule physisorbed on a spherical metal particle: nonlocal effects, C. Girard and F. Hache	118 (1987) 249
Multiphoton phenomena	
A photoelectron spectroscopy study of low-lying Rydberg states in molecular chlorine using multiphoton ionisation, B.G. Koenders, D.M. Wieringa, K.E. Drabe and C.A.	110 (1007) 113
de Lange Multiphoton ionization and fragmentation study of acetone at XeCl excimer laser	118 (1987) 113
radiation, H. Liu, S. Li, J. Han, Y. Guan and C. Wu	118 (1987) 285
Reactions (including dissociation)	
Investigations with the finite element method. II. The collinear $F + H_2$ reaction, R.	
Jaquet	118 (1987) 17
A generalized log-derivative method for the treatment of asymmetric collinear reac-	110 (1007) 205
tions in hyperspherical coordinates, F. Mrugala and J. Römelt	118 (1987) 295
– gas phase	
Monte Carlo simulation of RRKM unimolecular decomposition in molecular beam	
experiments. V. Product OX angular and energy distributions from $O(^3P) + X_2$	
(X = Br, I), P.A. Elofson, K. Rynefors and L. Holmlid	118 (1987) 1
Quantum-mechanical calculation of the reactions $D + FH(v = 0, 1, 2) \rightarrow DF(v') + H$	
and $H + FD(v = 0, 1, 2, 3) \rightarrow HF(v') + D$ on a realistic potential energy surface, J.A. Kaye, A. Kuppermann and J.P. Dwyer	118 (1987) 153
Magnetic field effects on atomic and molecular collisions, Y. Fukuda	118 (1987) 199
A theoretical study of the decomposition of halogenated alkoxy radicals. II. Fluorine	
extrusion, J.C. Rayez, M.T. Rayez, P. Halvick, B. Duguay and J.J. Dannenberg Rate constants for reactions $O(^3P) + X_2 \rightarrow OX + X$ (X = Br,I) determined by an	118 (1987) 265
RRKM-type statistical algorithm employing Monte Carlo simulation, K. Rynefors,	110 (1007) 417
L. Holmlid and P.A. Elofson	118 (1987) 417

The PF(A <sup>3</sup> Π-X <sup>3</sup> Σ <sup>-</sup> ) spectrum from He(2 <sup>3</sup> S) + PF <sub>3</sub> : extended vibrational analysis and PF(A) vibrational populations, U.K. Roychowdhury, S. Naxakis, J.A. Coxon, D.S. Richards, DZ. Cao and D.W. Setser	118 (1987) 427
-condensed phase  Evidence for solute-solute interactions in the inhibition of positronium in aqueous solutions, F.A. Smith and M.K. Pickard	118 (1987) 445
<ul> <li>- photochemical</li> <li>UV photoelectron spectroscopic study of the photopolymerization of long-chain diacetylene monocarboxylic acid in Langmuir-Blodgett films, H. Nakahara, K. Fukuda, K. Seki, S. Asada and H. Inokuchi</li> <li>Two-photon formation of NH/ND(A³Π) in the 193 nm photolysis of ammonia. I.</li> </ul>	118 (1987) 123
Mechanism and identification of the intermediate species, R.D. Kenner, F. Rohrer, R.K. Browarzik, A. Kaes and F. Stuhl Fluorescence lifetime studies of NO A <sup>2</sup> $\Sigma^+(v=5, N=9)$ , B <sup>2</sup> $\Pi_{3/2}(v=8, J=8.5)$ , C <sup>2</sup> $\Pi_{3/2}(v=1, J=8.5)$ , D <sup>2</sup> $\Sigma^+(v=0, N=5)$ and d <sup>2</sup> $\Sigma^+(v=1, N=9)$ , T. Hikida,	118 (1987) 141
T. Suzuki and Y. Mori  Tunnelling	118 (1987) 437
Study of the one-channel resonance states. Method without a stabilization procedure in the framework of the optical potential model, G. Jolicard and J. Humbert	118 (1987) 397
Positron annihilation Evidence for solute-solute interactions in the inhibition of positronium in aqueous solutions, F.A. Smith and M.K. Pickard	118 (1987) 445
Ionization (including Rydberg states) Multiphoton ionization and fragmentation study of acetone at XeCl excimer laser radiation, H. Liu, S. Li, J. Han, Y. Guan and C. Wu	118 (1987) 285
Molecular motion (including diffusive)  Vibrational dephasing under fractional ("stretched") exponential modulation in a liquid crystal system, W.G. Rothschild, R.M. Cavagnat and M. Perrot Coupling of the overall molecular motion with the conformational transitions. I. The	118 (1987) 33
model system of two coupled rotors, G. Moro Coupling of the overall molecular motion with the conformational transitions. II. The	118 (1987) 167
full rotational problem, G. Moro	118 (1987) 181
Isotopic effects  Quantum-mechanical calculation of the reactions $D + FH(v = 0, 1, 2) \rightarrow DF(v') + H$ and $H + FD(v = 0, 1, 2, 3) \rightarrow HF(v') + D$ on a realistic potential energy surface,  J.A. Kaye, A. Kuppermann and J.P. Dwyer	118 (1987) 153
Thermodynamic and transport properties  Thermodynamic excess properties from perturbation theory. Coupling-parameter approach, K.P. Shukla and J.M. Haile	118 (1987) 241
Structure of solids and liquids Gas-phase solvation of Cl <sup>-</sup> with H <sub>2</sub> O, CH <sub>3</sub> OH, C <sub>2</sub> H <sub>5</sub> OH, <i>i</i> -C <sub>3</sub> H <sub>7</sub> OH, <i>n</i> -C <sub>3</sub> H <sub>7</sub> OH, and <i>t</i> -C <sub>4</sub> H <sub>9</sub> OH, K. Hiraoka and S. Mizuse	118 (1987) 457

